

The embodiments of the invention in which an exclusive property or privilege is claimed are defined as follows:

1. Apparatus for creating a database containing the results of crystallization trials, said apparatus comprising:

an observation system for observing the results of crystallization trials;

a data input system for inputting the results of observing crystallization trials and related information; and

a database generator coupled to said data input system for receiving the results of observing crystallization trials and related information and creating a database for storing the results of observing crystallization trials and related information.

2. The apparatus claimed in Claim 1 wherein said observation system includes an optical system for observing a plurality of trays each including the results of a crystallization trial and a positioning system for selectively positioning a tray of said plurality of trays in an observation position.

3. The apparatus claimed in Claim 2 wherein said positioning system is coupled to and controlled by said database generator.

4. The apparatus claimed in Claim 1 wherein said data input system includes a microphone for receiving verbal data.

5. The apparatus claimed in Claim 4 wherein said data input system includes a feedback speaker for producing said verbal data as it is spoken.

6. The apparatus claimed in Claim 5 wherein said data input system includes a bar code scanner.

7. The apparatus claimed in Claim 1, wherein said data input system includes a display for displaying the data as pictographs on the display.

8. The apparatus claimed in Claim 1, wherein said data generator includes a programmed data processor for processing the results of observing crystallization trials and other information and a storage system for storing the results of said processing.

9. The apparatus claimed in Claim 8 wherein said programmed data processor includes a program having a plurality of database managers.

10. The apparatus claimed in Claim 9, wherein said plurality of database managers include:

a new trial manager for managing information relating to a crystallization trial set up.

11. The apparatus claimed in Claim 10, wherein the new trial manager includes a drop composition builder to capture information relating to crystallization drop components.

12. The apparatus claimed in Claim 11, wherein the new trial manager includes a normal trial builder.

13. The apparatus claimed in Claim 12, wherein the normal trial builder includes a copy wells builder to capture well condition information from a single matrix of crystallants.

14. The apparatus claimed in Claim 11, wherein the new trial manager includes a complex trial builder.

15. The apparatus claimed in Claim 14, wherein the complex trial builder includes a copy wells builder to capture well condition information from a plurality of matrices having crystallants.

16. The apparatus claimed in Claim 11, wherein the new trial manager includes a combinatorial trial builder.

17. The apparatus claimed in Claim 16, wherein the combinatorial trial builder includes a copy wells builder to capture well condition information in quad form.

18. The apparatus claimed in Claim 10, further comprising an existing trial manager to manage information relating to an existing trial.

19. The apparatus claimed in Claim 18, wherein the existing trial manager includes a drop composition calculator.

20. The apparatus claimed in Claim 18, wherein the existing trial manager includes a trial observation recording builder to capture crystallization trial results.

21. The apparatus claimed in Claim 20, wherein the trial observation recording builder includes a speech recognition builder for providing options for structuring verbal data input.

22. The apparatus claimed in Claim 21, wherein the speech recognition builder includes a voice command builder for customizing voice commands to include descriptors.

23. The apparatus claimed in Claim 22, wherein the voice command builder includes user definable voice commands for recognizing any one of a plurality of voice commands.

24. The apparatus claimed in Claim 10, further comprising a solution manager to manage information relating to solutions.

25. The apparatus claimed in Claim 24, wherein the solution manager includes a solution builder to capture information relating to a solution.

26. The apparatus claimed in Claim 25, wherein the solution includes a chemical selected from the group consisting of buffering agent, chelators, cryocoolants, CSIs, detergents, gases, heavy atom compounds, metals, nucleation suppressants, organic compounds, pH conjugates, precipitants, reducing agents, salts or solvents.

27. The apparatus claimed in Claim 25, wherein the solution builder can build a solution selected from the group consisting of additive, formulation, heavy atom, stock or buffer solutions.

28. The apparatus claimed in Claim 10, further comprising a matrix manager to manage information relating to a matrix of crystallant conditions.

29. The apparatus claimed in Claim 28, wherein the matrix manager includes a stock solution volume calculator to create new stock solutions for use in building matrices.

30. The apparatus claimed in Claim 29, wherein the matrix manager includes a new matrix builder to capture data relating to a new matrix of crystallants.

31. The apparatus claimed in Claim 10, further comprising a compound buffer manager to manage information relating to compound buffer systems.

32. The apparatus claimed in Claim 31, wherein the compound buffer manager includes a new compound buffer builder to capture data relating to a buffering system.

33. The apparatus claimed in Claim 10, further comprising a chemical manager to manage information relating to chemicals.

34. The apparatus claimed in Claim 33, wherein the chemical manager includes a chemical builder to capture data relating to chemicals relating to crystallization trials.

35. The apparatus claimed in Claim 34, wherein the chemical is selected from the group consisting of buffering agents, chelators, cryocoolants, CSIs, detergents, gases, heavy atom compounds, metals, nucleation suppressants, organic compounds, pH conjugates, precipitants, reducing agents, salts or solvents or any combination thereof.

36. The apparatus claimed in Claim 10, further comprising an apparatus manager to manage information relating to an apparatus used in a crystallization trial environment.

37. The apparatus claimed in Claim 36, wherein the apparatus manager includes a new apparatus builder for capturing data relating to a new crystallization plate.

38. The apparatus claimed in Claim 37, wherein the new apparatus builder includes an automatic fill wells builder for capturing information relating to the crystallization plate.

39. The apparatus claimed in Claim 37, wherein the new apparatus builder includes a manual fill wells builder for capturing information relating to the crystallization plate.

40. The apparatus claimed in Claim 36, wherein the apparatus manager includes an update apparatus builder for capturing information relating to an existing apparatus.

41. The apparatus claimed in Claim 10, further comprising a subunit manager for managing information relating to a macromolecule subunit.

42. The apparatus claimed in Claim 41, wherein the subunit manager includes a new subunit builder for capturing information relating to a new macromolecule subunit.

43. The apparatus claimed in Claim 41, wherein the subunit manager includes an update subunit builder for capturing information relating to an existing macromolecule subunit.

44. The apparatus claimed in Claim 41, wherein the subunit is from the class selected from the group consisting of proteins, DNA, RNA, protein-DNA complexes, protein-RNA complexes, DNA duplexes, RNA duplexes, DNA-RNA duplexes, glycoproteins, phosphoproteins, membrane proteins or any combination thereof.

45. The apparatus claimed in Claim 10, further comprising a macromolecule manager for managing information relating to a macromolecule relating to a crystallization trial.

46. The apparatus claimed in Claim 45, wherein the macromolecule manager includes a new macromolecule builder for capturing information relating to a new macromolecule relating to a crystallization trial.

47. The apparatus claimed in Claim 45, wherein the macromolecule is from the class selected from the group consisting of proteins, DNA, RNA, protein-DNA complexes, protein-RNA complexes, DNA duplexes, RNA duplexes, DNA-RNA duplexes, glycoproteins, phosphoproteins, membrane proteins or any combination thereof.

48. The apparatus claimed in Claim 10, further comprising a macromolecule formulation manager for managing macromolecule formulations relating to a crystallization trial.

49. The apparatus claimed in Claim 48, wherein the macromolecule formulation manager includes a new macromolecule formulation builder for capturing information relating to a macromolecule formulation.

50. The apparatus claimed in Claim 10, further comprising a complex macromolecule formulation manager for managing information relating to a complex macromolecule formulation relating to a crystallization trial.

51. The apparatus claimed in Claim 50, wherein the complex macromolecule formulation manager includes a new complex macromolecule formulation builder for capturing information relating to a complex macromolecule formulation.

52. The apparatus claimed in Claim 10, further comprising a manufacturer manager for managing information relating to manufacturers of chemicals and apparatuses relating to crystallization trials.

53. The apparatus claimed in Claim 52, wherein the manufacturer manager includes a new manufacturer builder to capture information relating to a new manufacturer.

54. The apparatus claimed in Claim 52, wherein the manufacturer manager includes an update manufacturer builder to capture information relating to an existing manufacturer.

55. The apparatus claimed in Claim 10 further comprising a collaborator manager to manage information relating to a collaborator.

56. The apparatus claimed in Claim 55, wherein the collaborator manager includes a new collaborator builder to capture information relating to a new collaborator.

57. The apparatus claimed in Claim 55, wherein the collaborator manager includes an update collaborator builder for capturing information relating to an existing collaborator.

58. The apparatus claimed in Claim 10, further comprising a project manager for managing information relating to a project.

59. The apparatus claimed in Claim 58, wherein the project manager includes a new project builder for capturing information relating to a new project.

60. The apparatus claimed in Claim 58, wherein the project manager includes an update project builder for capturing information relating to an existing project.

61. The apparatus claimed in Claim 10, further comprising a user manager for managing information relating to a user associated with a crystallization trial.

62. The apparatus claimed in Claim 61, wherein the user manager includes a new user builder for capturing information relating to a new user associated with a crystallization trial.

63. The apparatus claimed in Claim 61, wherein the user manager includes an update user builder to capture information relating to an existing user of a crystallization trial.

64. A computer implementable method of creating a database of crystallization trials and related information, said method comprising:

receiving via a dialog window, trial data, said trial data including information regarding the crystallization conditions to be used in a crystallization trial;

storing said received trial data in the database;

receiving, via a verbal input device, crystallization result data, said data including crystal type, crystal size, crystal shape, and crystal count; and

storing said received crystallization result data in the database.

65. The method claimed in Claim 64, further comprising:

receiving, via a dialog window, solution data, said solution data including solution type selected from the group consisting of additive, formulation, heavy atom, buffer solution, or stock solution; and

storing said solution data in the database.

66. The method claimed in Claim 64, further comprising:

receiving, via a dialog window, matrix data, said matrix data including matrix well conditions; and

storing said matrix data in a database.

67. The method claimed in Claim 64, further comprising:

receiving, via a dialog window, chemical data, said chemical data including chemical category selected from the group consisting of buffering agents, chelators, cryocoolants, CSIs, detergents, gasses, heavy atom compounds, metals, nucleation suppressants, organics, pH conjugates, precipitants, reducing agents, salts, or solvents; and

storing said chemical data in the database.

68. The method claimed in Claim 64, further comprising:

receiving, via a dialog window, apparatus data, said apparatus data including drop chamber coordinates, reservoir chamber coordinates, drop chamber diameter, reservoir chamber diameter, drop chamber maximum volume, and reservoir chamber maximum volume;

and storing said apparatus data in the database.

69. The method claimed in Claim 64, further comprising:

receiving via a dialog window, subunit data, said subunit data including subunit class selected from the group consisting of proteins, DNAs, RNAs, protein-DNA complexes, protein-RNA complexes, DNA duplexes, RNA duplexes, DNA-RNA duplexes, glycoproteins, phosphoproteins, membrane proteins or any combination thereof; and

storing said subunit data in the database.

70. The method claimed in Claim 64, further comprising macromolecule data, said macromolecule data including molecule class selected from the group consisting of proteins, DNAs, RNAs, protein-DNA complexes, protein-RNA complexes, DNA duplexes, RNA duplexes, DNA-RNA duplexes, glycoproteins, phosphoproteins, membrane proteins or any combinations thereof; and

storing said macromolecule data in the database.

71. A computer readable medium having a plurality of computer executable database managers for creating a database of the results of crystallization trials and related information, said database manager including:

a trial manager for entering into the database trial information.

72. The computer readable medium of Claim 71, further comprising a normal trial builder, a complex trial builder, and a combinatorial trial builder.

73. A computer readable medium having a plurality of computer executable database managers for creating a database of the results of crystallization trials and related information, said database manager including:

a matrix manager for entering into the database matrix information; and
a chemical manager for entering into the database chemical information.

74. The computer readable medium of Claim 73, further comprising a new matrix builder for entering new matrix information into the database.

75. The computer readable medium of Claim 73, further comprising a new chemical builder and an update chemical builder for entering new and updated chemical information.

76. A computer readable medium having a plurality of computer executable database managers for creating a database of the results of crystallization trials and related information, said database managers including:

an apparatus manager for entering into the database apparatus information;
and
a manufacturer manager for entering into the database manufacturer information.

77. The computer readable medium of Claim 76, further comprising a new and an update apparatus builder, for entering into the database new and updated apparatus information.

78. The computer readable medium of Claim 76, further comprising a new and an update manufacturer builder, for entering into the database new and updated manufacturer information.

79. A computer readable medium having a plurality of computer executable database managers for creating a database of the results of crystallization trials and related information, said database managers including:

a subunit manager for entering into the database subunit information.

80. The computer readable medium of Claim 79, further comprising a new and an update subunit builder, for entering into the database new and updated subunit information.

81. The computer readable medium of Claim 80 further including:
a macromolecule manager for entering into the database macromolecule information.
82. The computer readable medium of Claim 81, further including:
a new macromolecule builder for entering into the database new macromolecule information.
83. The computer readable medium of Claim 80 further including:
a macromolecule formulation manager for entering into the database macromolecule formulation information.
84. The computer readable medium of Claim 83, further including a new macromolecule formulation builder for entering into the database new macromolecule formulation information.
85. The computer readable medium of Claim 80 further including:
a complex macromolecule formulation manager for entering into the database complex macromolecule formulation information.
86. The computer readable medium of Claim 85, further including:
a new complex macromolecule formulation builder for entering into the database new complex macromolecule formulation information.
87. A computer readable medium having stored thereon a crystallization trial results data structure including at least the following fields:
a chemical type ID field;
a CAS field; and
a catalog field.
88. The computer readable medium of Claim 87, wherein the chemical type is selected from the group consisting of buffering agents, chelators, cryocoolants, CSIs, detergents, gasses, heavy atom compounds, metals, nucleation suppressants, organic compounds, pH conjugates, precipitants, reducing agents, salts, solvents, or any combination thereof.

89. A computer readable medium having stored thereon a crystallization trial results data structure as claimed in Claim 1, further including the following fields:

- crystal type;
- crystal size;
- crystal count; and
- crystal shape.

90. A computer readable medium having stored thereon a crystallization trial results data structure as claimed in Claim 89, further including the following field:

- macromolecule class ID.

91. The computer readable medium of Claim 90, wherein the macromolecule class is selected from the group consisting of proteins, DNAs, RNAs, protein-DNA complexes, protein-RNA complexes, DNA duplexes, RNA duplexes, DNA-RNA duplexes, glycoproteins, phosphoproteins, membrane proteins, or any combination thereof.

92. A computer readable medium having stored thereon a crystallization trial results data structure as claimed in Claim 89, further including the following field:

- session ID.